=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538.str

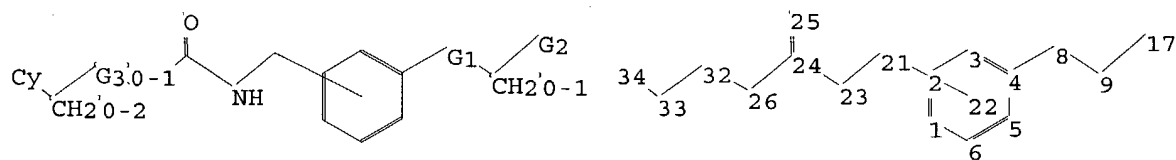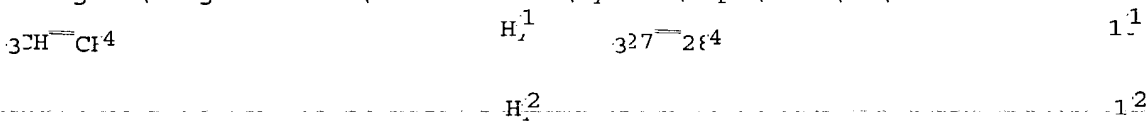3CH═Cl4   H1   327═2C4   11

                        H2   12

chain nodes :
8   9   10   11   17   21   23   24   25   26   27   28   32   33   34
ring nodes :
1   2   3   4   5   6
chain bonds :
4-8   8-9   9-17   21-23   23-24   24-25   24-26   26-32   27-28   32-33   33-34
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6
exact/norm bonds :
4-8   8-9   9-17   21-23   23-24   24-25   26-32   32-33   33-34
exact bonds :
24-26   27-28
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
containing 1 :

G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   8:CLASS   9:CLASS   10:Atom   11:Atom
17:CLASS   21:CLASS   22:CLASS   23:CLASS   24:CLASS   25:CLASS   26:CLASS   27:CLASS
28:CLASS   32:CLASS   33:CLASS   34:Atom
Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System   : Monocyclic
11:

Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic

Element Count :
Node 10: Limited
     C,C5
     N,N1
     S,S0
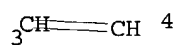   O,O0

Node 11: Limited
     C,C4
     N,N2
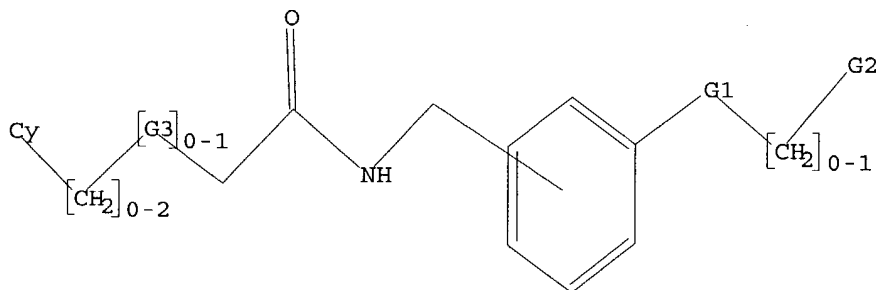   O,O0
     S,S0

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

$_3$CH=CH ^{4}

Hy ^{1}

Hy ^{2}

G1 O,N
G2 [@1],[@2]
G3 CH2,[@3-@4]

Structure attributes must be viewed using STN Express query preparation.


```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 18:47:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 115414 TO ITERATE

   0.9% PROCESSED    1000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0 ·

L2            0 SEA SSS SAM L1

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L3    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L4    SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (a).str
```
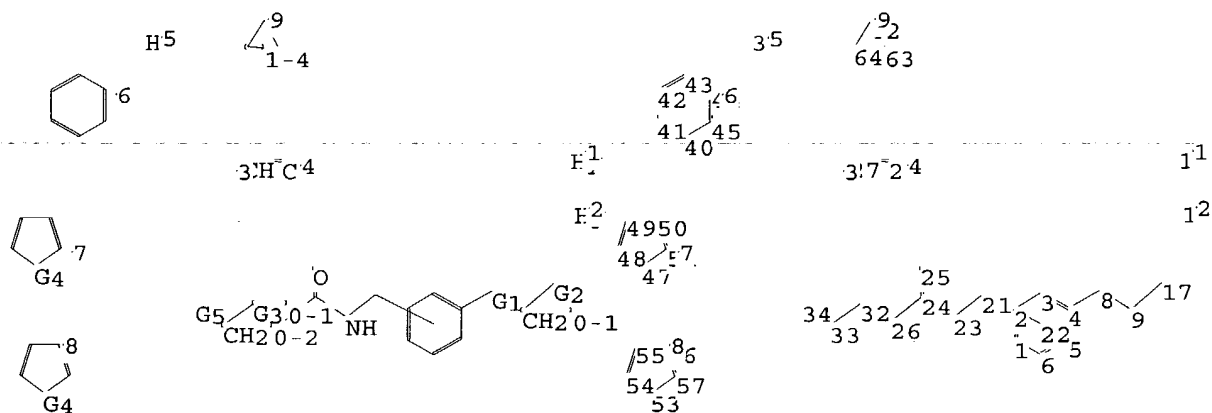
H⁵

⁹
1-4

3⁵

⁹
-2
6463

⁶

42⁄43 ⁄6
41⁄45
40

3.H C 4

F 1

3.7 2 4

1 1

1 2

7
G4

F 2
/4950
48⁄ 7.
4 7

O
G5⁄G3 0-1   NH   G1⁄G2
CH2 0-2   CH2 0-1

/55 8 6
54⁄57
53

25
34⁄32⁄24 ⁄21⁄3 ⁄8⁄17
33   26 23 2 4 9
1 22 5
6

8
G4

```
chain nodes :
8   9   10  11  17  21  23  24  25  26  27  28  32  33  34  39
ring nodes :
1   2   3   4   5   6   40  41  42  43  44  45  47  48  49  50  51  53  54  55  56  57
62  63  64
chain bonds :
4-8   8-9   9-17   21-23   23-24   24-25   24-26   26-32   27-28   32-33   33-34
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   40-41   40-45   41-42   42-43   43-44   44-45   47-48
47-51  48-49  49-50  50-51  53-54  53-57  54-55  55-56  56-57  62-63  62-64  63-64
exact/norm bonds :
4-8   8-9   9-17   21-23   23-24   24-25   24-26   26-32   27-28   32-33   33-34   47-48
47-51  48-49  49-50  50-51  53-54  53-57  54-55  55-56  56-57  62-63  62-64  63-64
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   40-41   40-45   41-42   42-43   43-44   44-45
isolated ring systems :
containing 1 : 40 : 47 : 53 :


G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]
```

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom 11:Atom
17:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 32:CLASS 33:CLASS 34:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom
44:Atom 45:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 62:Atom 63:Atom 64:Atom
Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System   : Monocyclic
11:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic
39:
Saturation   : Unsaturated
Number of Hetero Atoms : less than 2

Element Count :
Node 10: Limited
     C,C5
     N,N1
     S,S0
     O,O0

Node 11: Limited
     C,C4
     N,N2
     O,O0
     S,S0

Node 39: Limited
     C,C5-9
     N,N1
     O,O0
     S,S0

L5   STRUCTURE UPLOADED

=> que L5 AND L3 NOT L4

L6   QUE L5 AND L3 NOT L4

=> d l6
L6 HAS NO ANSWERS
L3   SCR 1840
L4   SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L5   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L6   QUE   L5 AND L3 NOT L4

```
=> s l6 sss sam
SAMPLE SEARCH INITIATED 18:53:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  80732 TO ITERATE

   1.2% PROCESSED    1000 ITERATIONS                        0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **INCOMPLETE**
                        BATCH    **INCOMPLETE**
PROJECTED ITERATIONS:     EXCEEDS 1000000
PROJECTED ANSWERS:        EXCEEDS        0

L7              0 SEA SSS SAM L5 AND L3 NOT L4

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L8    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L9    SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (b).str
```
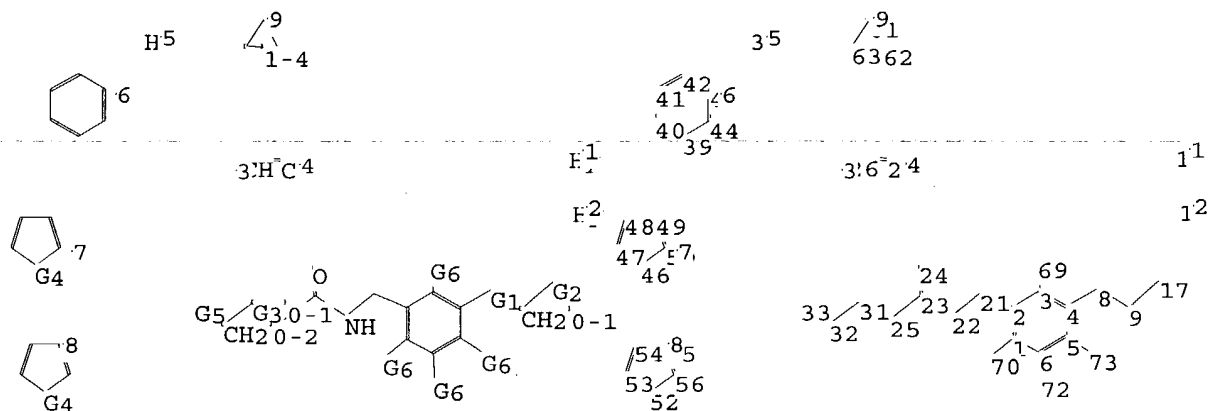
H 5

∠9
1-4

·6

3 5

∠91
6362

41 42 ·6
40 44
39

F 1

3:6 2 4

1 1

3:H C 4

F 2

48 49
47 F 7
46

1 2

G4 ·7

O

G6

G1 G2

24 69

33 31 23 21 2 3 8 17
32 25 22 4 9

G5 G3 0-1
CH2 0-2

NH

G6

CH2 0-1

G6

G6
G6

54 85
53 56
52

70 6 5 73
1 72

G4 ·8

chain nodes :
8   9   10   11   17   21   22   23   24   25   26   27   31   32   33   38   69   70   72   73
ring nodes :
1   2   3   4   5   6   39   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56
61   62   63
chain bonds :
1-70   2-21   3-69   4-8   5-73   6-72   8-9   9-17   21-22   22-23   23-24   23-25   25-31
26-27   31-32   32-33
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44   46-47
46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55   55-56   61-62   61-63   62-63
exact/norm bonds :
1-70   2-21   3-69   4-8   5-73   6-72   8-9   9-17   21-22   22-23   23-24   23-25   25-31
26-27   31-32   32-33   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
55-56   61-62   61-63   62-63
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44
isolated ring systems :
containing 1 : 39 : 46 : 52 :

G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom 11:Atom
17:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
31:CLASS 32:CLASS 33:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom
44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 61:Atom 62:Atom 63:Atom 69:CLASS 70:CLASS 72:CLASS 73:CLASS

Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System   : Monocyclic
11:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic
38:
Saturation   : Unsaturated
Number of Hetero Atoms : less than 2

Element Count :
Node 10: Limited
     C,C5
     N,N1
     S,S0
     O,O0

Node 11: Limited
     C,C4
     N,N2
     O,O0
     S,S0

Node 38: Limited
     C,C5-9
     N,N1
     O,O0
     S,S0

L10   STRUCTURE UPLOADED

=> que L10 AND L8 NOT L9

L11 QUE L10 AND L8 NOT L9

```
=> d l11
L11 HAS NO ANSWERS
L8              SCR 1840
L9              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L10             STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

```
Structure attributes must be viewed using STN Express query preparation.
L11             QUE  L10 AND L8 NOT L9


=> s l11 sss sam
SAMPLE SEARCH INITIATED 18:55:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2266 TO ITERATE

 44.1% PROCESSED    1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      42465 TO    48175
PROJECTED ANSWERS:             0 TO        0

L12            0 SEA SSS SAM L10 AND L8 NOT L9

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L13   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L14   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (d).str
```
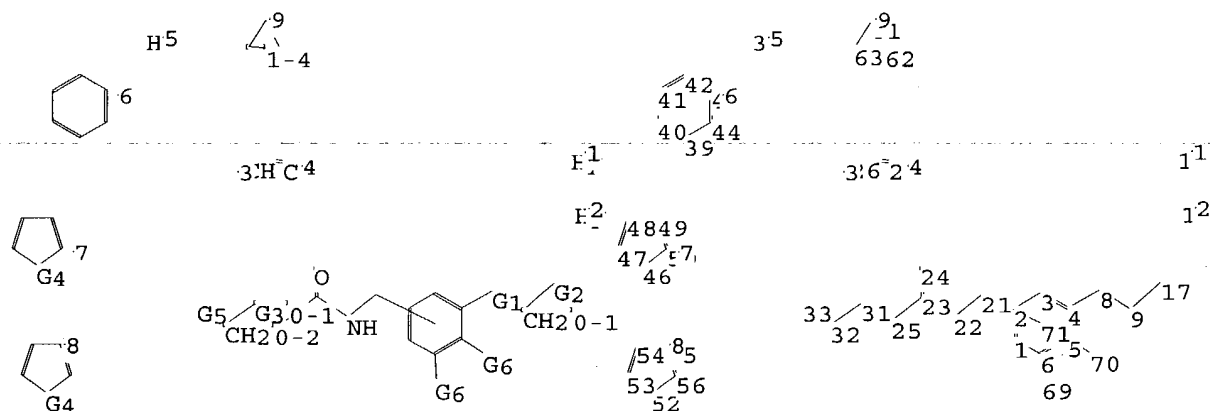
H`5`

∠`9`
1-4

3`5`

/`9`
`1`
6362

42
41/ ⟨6
40 ⟨44
39

`6`

3:H⁼C`4`

F`1`

3:6⁼2`4`

1`1`

F`2`

/4849
47/ε7⟩
46

12

`7`
G4

O
‖
G5\ /G3'0-1
CH2'0-2   NH

G1\ /G2
CH2'0-1

24
33/31/23/21\3\ 8\ /17
32 25 22 2\ /71\ /9
1\ /5\70
6 69

`8`
G4

G6

G6

/54 8`5`
53/ \56
52

69

```
chain nodes :
8   9   10   11   17   21   22   23   24   25   26   27   31   32   33   38   69   70
ring nodes :
1   2   3   4   5   6   39   40   41   42   43   44   46   47   48   49   50   52   53   54   55   56
61   62   63
chain bonds :
4-8   5-70   6-69   8-9   9-17   21-22   22-23   23-24   23-25   25-31   26-27   31-32   32-33
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44   46-47
46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55   55-56   61-62   61-63   62-63
exact/norm bonds :
4-8   5-70   6-69   8-9   9-17   21-22   22-23   23-24   23-25   25-31   26-27   31-32   32-33
46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55   55-56   61-62   61-63
62-63
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44
isolated ring systems :
containing 1 : 39 : 46 : 52 :


G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]
```

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom 11:Atom
17:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
31:CLASS 32:CLASS 33:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom
44:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 61:Atom 62:Atom 63:Atom 69:CLASS 70:CLASS 71:CLASS
Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System   : Monocyclic
11:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic
38:
Saturation   : Unsaturated
Number of Hetero Atoms : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 38: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0

L15   STRUCTURE UPLOADED

=> que L15 AND L13 NOT L14

L16   QUE L15 AND L13 NOT L14

=> d l16
L16 HAS NO ANSWERS

```
L13             SCR  1840
L14             SCR  2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L15             STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
```
L16             QUE  L15 AND L13 NOT L14
```


```
=> s l16 sss sam
SAMPLE SEARCH INITIATED 18:57:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  80732 TO ITERATE

   1.2% PROCESSED    1000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **INCOMPLETE**
                         BATCH    **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L17             0 SEA SSS SAM L15 AND L13 NOT L14

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1840

L18   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L19   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10719538 (e).str
```

chain nodes :
8   9   10 11 17 21 22 23 24 25 26 27 31 32 33 38 69 70 73 75 92
93 94 95 96 98 99 100 102
ring nodes :
1   2   3   4   5   6   39 40 41 42 43 44 46 47 48 49 50 52 53 54 55 56
61 62 63 76 77 78 79 80 81 82 83 84 85 86 87
chain bonds :
1-75   3-73   5-70   6-69   8-9   8-102   9-17   21-22   21-102   22-23   23-24   23-25   25-31
 26-27   31-32   32-33   76-94   77-93   78-92   81-95   82-99   84-98   85-96   87-100
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44   46-47
46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55   55-56   61-62   61-63   62-63
76-77   76-81   77-78   78-79   79-80   80-81   82-83   82-87   83-84   84-85   85-86   86-87
exact/norm bonds :
1-75   3-73   5-70   6-69   8-9   8-102   9-17   21-22   21-102   22-23   23-24   23-25   25-31
 26-27   31-32   32-33   46-47   46-50   47-48   48-49   49-50   52-53   52-56   53-54   54-55
 55-56   61-62   61-63   62-63   76-94   77-93   78-92   81-95   82-99   84-98   85-96
87-100
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   39-40   39-44   40-41   41-42   42-43   43-44   76-77
76-81   77-78   78-79   79-80   80-81   82-83   82-87   83-84   84-85   85-86   86-87
isolated ring systems :
containing 1 : 39 : 46 : 52 : 76 : 82 :

G1:O,N

G2:[*1],[*2]

G3:CH2,[*3-*4]

G4:O,S

G5:[*5],[*6],[*7],[*8],[*9]

G6:H,Cl,Br,F,I

G7:[*10-*11],[*12-*13],[*14-*15]

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   8:CLASS   9:CLASS   10:Atom   11:Atom
17:CLASS   21:CLASS   22:CLASS   23:CLASS   24:CLASS   25:CLASS   26:CLASS   27:CLASS
31:CLASS   32:CLASS   33:Atom   38:Atom   39:Atom   40:Atom   41:Atom   42:Atom   43:Atom
44:Atom   46:Atom   47:Atom   48:Atom   49:Atom   50:Atom   52:Atom   53:Atom   54:Atom
55:Atom   56:Atom   61:Atom   62:Atom   63:Atom   69:CLASS   70:CLASS   73:CLASS   75:CLASS
 76:Atom   77:Atom   78:Atom   79:Atom   80:Atom   81:Atom   82:Atom   83:Atom   84:Atom
85:Atom   86:Atom   87:Atom   92:CLASS   93:CLASS   94:CLASS   95:CLASS   96:CLASS
98:CLASS   99:CLASS   100:CLASS   102:CLASS
Generic attributes :
10:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System   : Monocyclic
11:
Saturation   : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System   : Monocyclic
38:
Saturation   : Unsaturated
Number of Hetero Atoms : less than 2

Element Count :
Node 10: Limited
    C,C5
    N,N1
    S,S0
    O,O0

Node 11: Limited
    C,C4
    N,N2
    O,O0
    S,S0

Node 38: Limited
    C,C5-9
    N,N1
    O,O0
    S,S0

L20   STRUCTURE UPLOADED

=> que L20 AND L18 NOT L19

L21   QUE L20 AND L18 NOT L19

=> d l21
L21 HAS NO ANSWERS
L18   SCR 1840
L19   SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L20   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L21   QUE L20 AND L18 NOT L19

=> s l21 sss sam
SAMPLE SEARCH INITIATED 19:01:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 16543 TO ITERATE

   6.0% PROCESSED   1000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 323163 TO   338557
PROJECTED ANSWERS: 0 TO   0

L22   0 SEA SSS SAM L20 AND L18 NOT L19

=> s l21 sss ful
FULL SEARCH INITIATED 19:01:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 330291 TO ITERATE

100.0% PROCESSED 330291 ITERATIONS   7 ANSWERS
SEARCH TIME: 00.00.09

L23   7 SEA SSS FUL L20 AND L18 NOT L19

=> => s l23
L24   2 L23

=> d l24 1-2 bib,ab,hitstr

L24 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN   1998:268482 CAPLUS
DN   128:321930
TI   Preparation of β-thiopropionylamino acid derivatives as
     β-lactamase inhibitors
IN   Bateson, John Hargreaves; Best, Desmond John; Clarke, Brian Peter; Gilpin,
     Martin Leonard; Witty, David R.; et al.
PA   Smithkline Beecham Plc, UK; Bateson, John Hargreaves; Best, Desmond John;
     Clarke, Brian Peter; Gilpin, Martin Leonard
SO   PCT Int. Appl., 98 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
         PATENT NO.   KIND DATE   APPLICATION NO.   DATE
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PI   WO 9817639   A1   19980430   WO 1997-EP5709   19971010
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG,
             US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     AU 9850501   A1   19980515   AU 1998-50501   19971010
     EP 934262   A1   19990811   EP 1997-913147   19971010
         R: BE, CH, DE, ES, FR, GB, IT, LI, NL
     JP 2001502345   T2   20010220   JP 1998-518931   19971010
     US 6156774   A   20001205   US 1999-284098   19990407
PRAI GB 1996-21692   A   19961017
     GB 1997-4581   A   19970305
     GB 1997-16212   A   19970731
     WO 1997-EP5709   W   19971010
OS   MARPAT 128:321930
AB   Title mercapto amino acid derivs. R4SCR5R6CHR3CONR2CHR1CO2R [I; R = H,
     salt-forming cation of in vivo hydrolyzable ester-forming group; R1 = Q,
     Q1; ring A = monocyclic aryl or heteroaryl ring; ring B = monocyclic aryl,
     alicyclic, or heterocyclic ring; C, D = Zp(CR8CR9)q, (CR8CR9)qZp; p = 0,
     1, q = 0-3 provided that p + q ≠ 0 in C; R8, R9 = H, (C1-6)alkyl;
     CR8R9 = O; Z = O, NR10, S(O)x; R10 = H, (C1-6)alkyl. aryl(C1-6)alkyl; x =
     0-2; wherein C and D are linked ortho to one another on each of the rings
     A and B in Q1; R2 = H, (C1-6)alkyl, aryl(C1-6)alkyl; R3 = H, (C1-6)alkyl
     substituted by 0-3 halo atoms, (C3-7)cycloalkyl, fused
     aryl(C3-7)cycloalkyl, (C3-7)cycloalkyl(C2-6)alkyl, (C2-6)alkenyl,
     (C2-6)alkynyl, aryl, aryl-(CH2)m-X-(CH2)n, heterocyclyl,
     heterocyclyl-(CH2)m-X-(CH2)n; m = 0-3; n = 1-3; X = O, S(O)x, bond; R4 = H
     or in vivo hydrolyzable acyl; R5, R6 = H, (C1-6)alkyl; R5R6 = (CH2)2-5]
     for use in treatment of bacterial infections in humans or animals by
     administration in combination with a β-lactam antibiotic. Thus,
     lithiation of thiophene and alkylation with 3-(bromomethyl)tetrahydrofuran
     gave 2-(tetrahydrofuran-3-ylmethyl)thiophene, which underwent lithiation
     and acylation with Et oxalyl chloride to give oxoacetate II (X1 = O). II
     (X1 = O) was converted into hydroxyiminoacetate II (X1 = NOH), reduced in
     situ to the corresponding amine, acylated with 2-(acetylthio)4-
     phenylbutanoic acid (preparation given), and saponified to give desired title
     compound III. III and related mercaptopropionyl derivs. inhibited
     Bacteroides fragilis CfiA metallo-β-lactamase with IC50 <1 µM.
     Compound III inhibited Bacteroides fragilis 262 strain, which produces CfiA
     metallo-β-lactamase, alone with MIC >256 µg/mL, but with MIC 16

μg/mL in the presence of 8 μg/mL meropenem.

IT   **206765-11-9P 206765-12-0P 206765-13-1P**
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
     (preparation of β-thiopropionylamino acid derivs. as β-lactamase
     inhibitors)

RN   206765-11-9 CAPLUS
CN   Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-
     phenylbutyl]amino]-4-(4-pyridinylmethoxy)-, (αR)-(9CI)   (CA INDEX
     NAME)

Absolute stereochemistry.
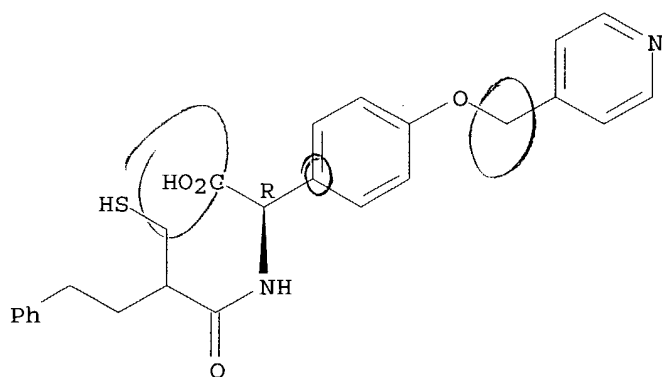
RN   206765-12-0 CAPLUS
CN   Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-
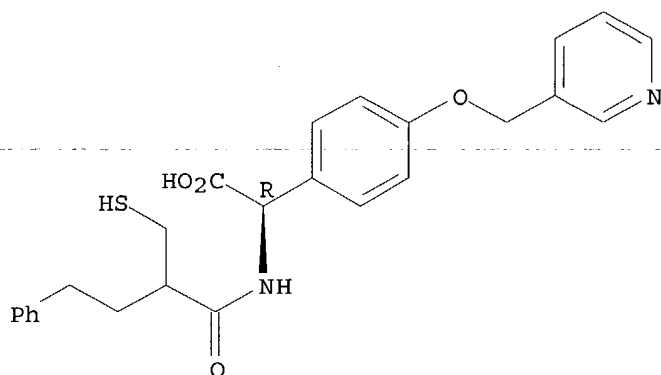   phenylbutyl]amino]-4-(2-pyridinylmethoxy)-, (αR)-(9CI)   (CA INDEX
     NAME)

Absolute stereochemistry.
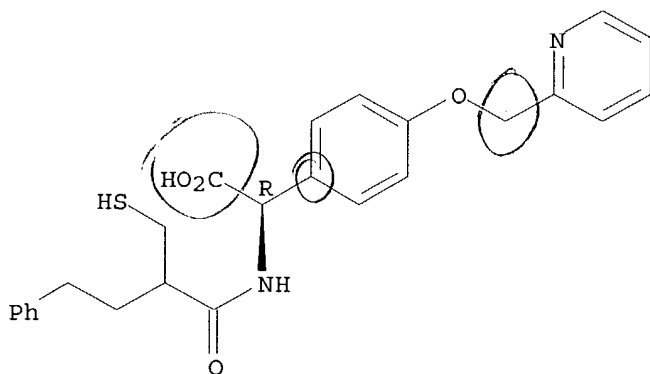
RN   206765-13-1 CAPLUS
CN   Benzeneacetic acid, α-[[2-(mercaptomethyl)-1-oxo-4-
     phenylbutyl]amino]-4-(3-pyridinylmethoxy)-, (αR)-(9CI)   (CA INDEX
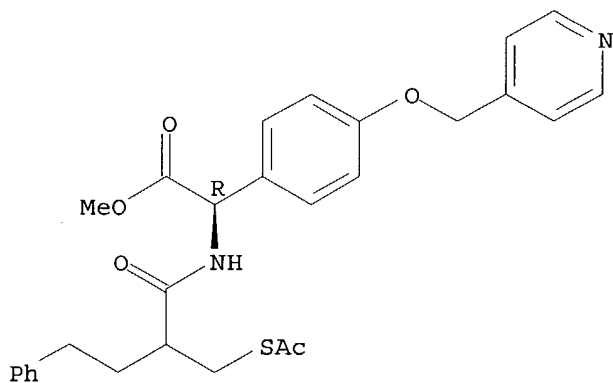   NAME)

Absolute stereochemistry.

IT   **206766-05-4P 206766-06-5P 206766-07-6P**
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
          (preparation of β-thiopropionylamino acid derivs. as β-lactamase
          inhibitors)
RN   206766-05-4 CAPLUS
CN   Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-
     phenylbutyl]amino]-4-(4-pyridinylmethoxy)-, methyl ester, (αR)-
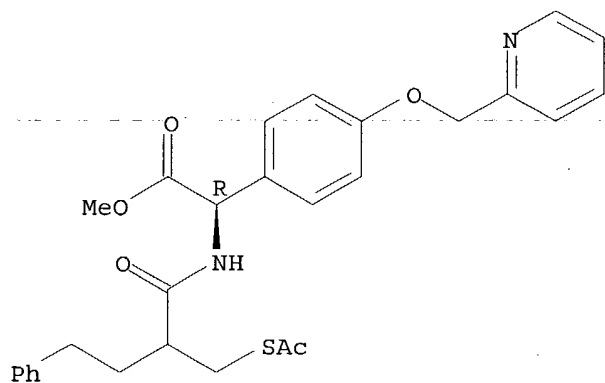   (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   206766-06-5 CAPLUS
CN   Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-
     phenylbutyl]amino]-4-(2-pyridinylmethoxy)-, methyl ester, (αR)-
     (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   206766-07-6 CAPLUS
CN   Benzeneacetic acid, α-[[2-[(acetylthio)methyl]-1-oxo-4-
       phenylbutyl]amino]-4-(3-pyridinylmethoxy)-, methyl ester, (αR)-
       (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
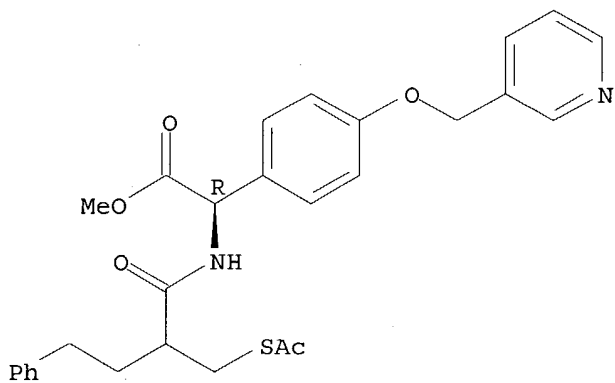

RE.CNT 6   THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
                 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24   ANSWER 2 OF 2   CAPLUS   COPYRIGHT 2004 ACS on STN
AN   1996:271992   CAPLUS
DN   125:59045
TI   Multipin solid phase synthesis of ethers using modified Mitsunobu
       chemistry
AU   Valerio, Robert M.; Bray, Andrew M.; Patsiouras, Heather
CS   Chiron Mimotypes Pty. Ltd., Clayton, 3169, Australia
SO   Tetrahedron Letters (1996), 37(17), 3019-22
       CODEN: TELEAY; ISSN: 0040-4039
PB   Elsevier
DT   Journal
LA   English
AB   Formation of ether derivs. of phenolic containing structures using solid phase
       Mitsunobu chemical on functionalized polyethylene pins was investigated.
       Using the multipin approach, a range of reaction parameters were
       systematically varied in parallel expts. including solvent, temperature, time,
       reactant concns., base, phosphine and alc. to determine optimum reaction
       conditions. Solid phase reaction of three phenols with a range of alcs.
       to form the ethers proceeds smoothly using 0.15M PPh3/DEAD/alc. in THF at
       37° for 4 days in the presence of 0.45M Et3N.
IT   **178119-96-5P**
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (multipin solid phase synthesis of aryl ethers using modified Mitsunobu
          chemical)
RN   178119-96-5 CAPLUS
CN   Glycinamide, N-[(4-methylphenyl)acetyl]-D-2-[4-(3-
       pyridinylmethoxy)phenyl]glycyl- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
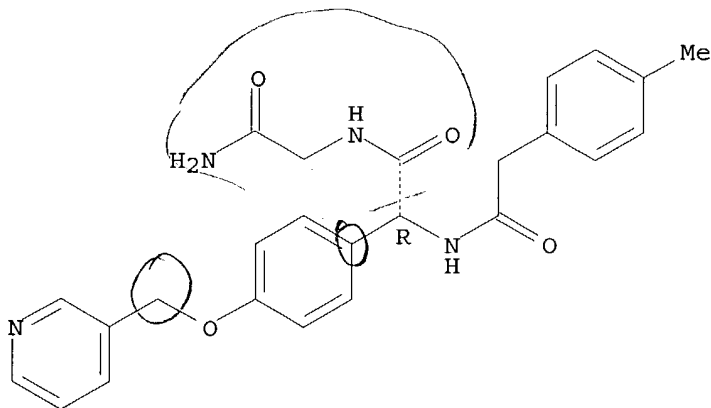
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L3              SCREEN 1840
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L5              STRUCTURE UPLOADED
L6              QUE L5 AND L3 NOT L4
L7          0 S L6 SSS SAM
L8              SCREEN 1840
L9              SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L10             STRUCTURE UPLOADED
L11             QUE L10 AND L8 NOT L9
L12         0 S L11 SSS SAM
L13             SCREEN 1840
L14             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
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L16             QUE L15 AND L13 NOT L14
L17         0 S L16 SSS SAM
L18             SCREEN 1840
L19             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
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L21             QUE L20 AND L18 NOT L19
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L23         7 S L21 SSS FUL

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE       TOTAL
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CA SUBSCRIBER PRICE                              0.00         -1.39

STN INTERNATIONAL LOGOFF AT 19:02:28 ON 08 APR 2004
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